Anomalous Scattering by Subwavelength Slit Structures and their applications

Hai Zhang

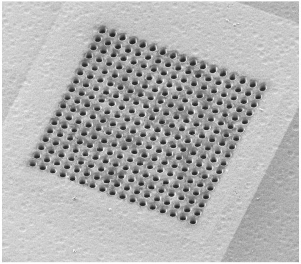
Department of Mathematics, HKUST

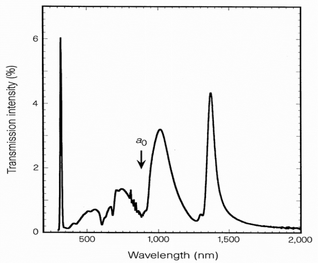
11-th Zurich Summer School, Aug 23-27, 2021

Extraordinary Optical Transmission Through a Small Hole Array

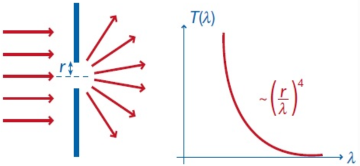
T. W. Ebbessen *et al*, Nature (1998)

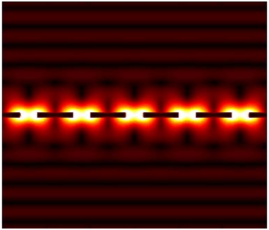
Size of each hole: 150 nm, metal thickness: 300 nm, skin depth: 30nm





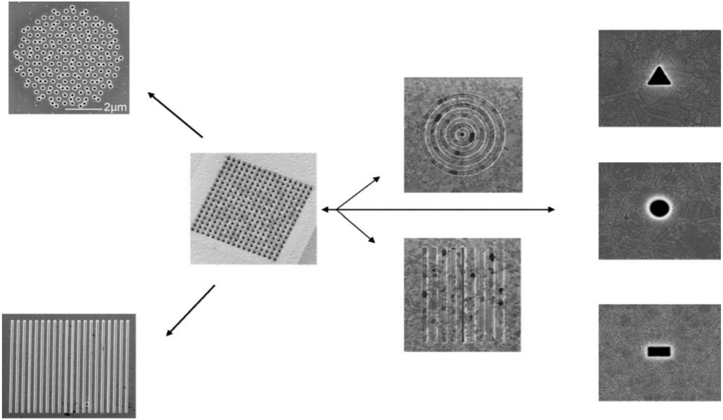
Classical Bethe theory for diffraction by a small hole





Subsequent Development in Extraordinary Optical Field Enhancement

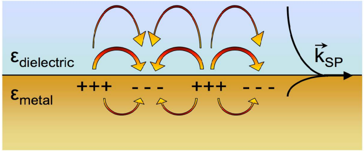
F. J. Garcia-Vidal *et al*, Rev. Mod. Phy. (2010)
S. Rodrigo, F. León-Pérez, L. Martín-Moreno, Proceedings of the IEEE (2016)

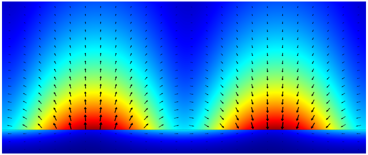


Applications: Near-field optical imaging, biosensing, novel optical devices....

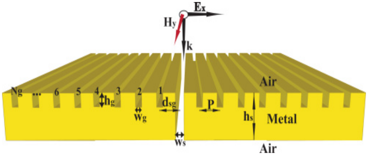
Possible Enhancement Mechanisms

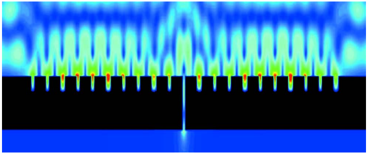
- Surface plasmonic resonances in noble metals





- Non-plasmonic resonances (e.g., resonances induced by the geometry of the structure)



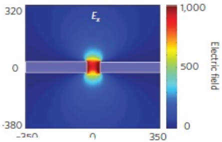


- Surface waves.
- other enhancement mechanism?

Questions

- There has been a long debate on the interpretation of enhancement effects. For instance, surface plasmonic resonances strengthen or inhibit the enhancement? interplay between different enhancement mechanisms?
- Other questions: How large is the enhancement and at what frequencies?
- Quantitative analysis of the field enhancement would be desirable!
- Efficient numerical modeling techniques, optimal design for better performance.

Outline of the lectures



Slit structures in perfect conducting (PEC) metals:

- Lecture 1: Resonant and non-resonant enhancement effects for a single slit and an array of slits in the diffraction regime.
- Lecture 2: Enhancement effects for an array of slits in the homogenization regime; "surface spoof plasmon" and total transmission; Fano resonance.
- Lecture 3: Applications in super-resolution imaging and sensing.

Our main approach and related work

- Mathematical tools:
  - layer potential techniques;
  - Gohberg-Sigal theory: reduce the problem of resonances/eigenvalues to the characteristic values of operator-valued functions, and to the roots of complex-valued functions;
  - Asymptotic analysis to boundary integral operators.
  - Reference book: Mathematical and Computational Methods in Photonics and Phononics. H. Ammari, B. Fitzpatrick, H. Kang, M. Ruiz, S. Yu, and Z, Mathematical Surveys and Monographs, Volume 235, AMS, 2018.

Related mathematical work:

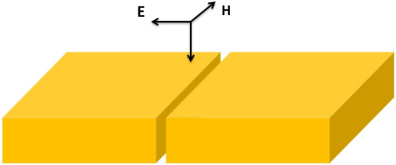
- E. Bonnetier and F. Triki (2010): Asymptotics of the Green function for a subwavelength cavity.
- Plasmonic waves allow perfect transmission through sub-wavelength metallic gratings, G. Bouchitté, B. Schweizer, 2012.
- P. Joly and S. Tordeux, Matched asymptotic expansion, 2006, 2008.

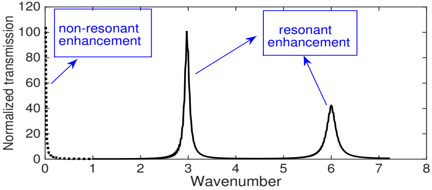
Lecture 1-1: Anomalous Scattering by a Single Subwavelength Slit Structures

Joint work with Junshan Lin, Auburn University

Scattering and field enhancement of a perfect conducting narrow slit
SIAM Journal on Applied Math, 2017

Electromagnetic Field Enhancement in a Single PEC Slit





Transmission with metal thickness = 1, gap size = 0.02.

- Resonant effect

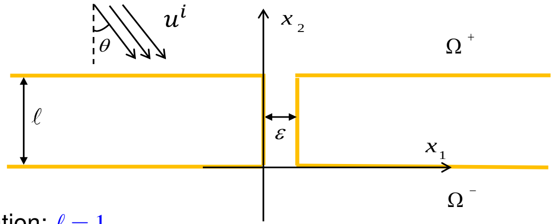
  Y. Takakura (2001), J. Sambles *et al* (2002), F. Garcia-Vidal, *et al* (2004), R. Gordon (2006) $\cdots$

- Non-resonant effect

  Experiments: D-S. Kim (2009), S-H. Oh (2014)

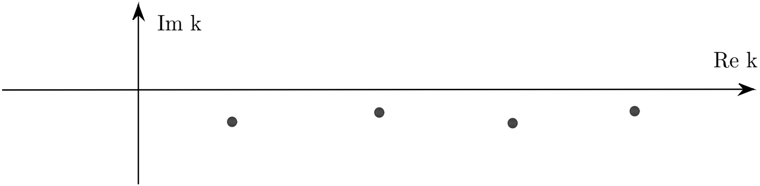
Answer the following questions:

- What are the resonant frequencies?
- Can one characterize the wave modes at resonant frequencies?
- What induces the enhancement at non-resonant frequencies?



- Normalization: $\ell = 1$.
- The exterior domain: $\Omega_\varepsilon = \Omega_+ \cup \Omega_- \cup S_\varepsilon$.
- TM polarization: the incident magnetic field $H^i = (0, 0, u^i)$, where $u^i = e^{ikd\cdot x}$, $k = \omega/c$.
- The total field $u_\varepsilon = u^i + u^r + u^s_\varepsilon$ in Ω^+, and $u_\varepsilon = u^s_\varepsilon$ (transmitted wave) in Ω^-.
- The scattering problem:

$$\begin{cases} \Delta u_\varepsilon + k^2 u_\varepsilon = 0 & \text{in } \Omega_\varepsilon, \\ \dfrac{\partial u_\varepsilon}{\partial \nu} = 0 & \text{on } \partial\Omega_\varepsilon. \\ \lim\limits_{r\to\infty} \sqrt{r}\left(\dfrac{\partial u^s_\varepsilon}{\partial r} - iku^s_\varepsilon\right) = 0, & r = |x|. \end{cases}$$

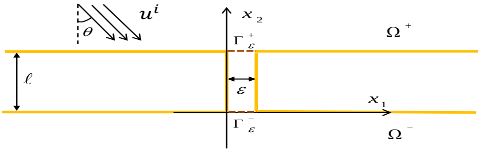


- Fact: The scattering problem attains a unique solution if Im $k \geq 0$.

Defintion

The *scattering resonances* are the poles of the scattering operator when continued meromorphically to the whole complex plane.

- Field enhancement at resonant frequencies: $O\left(\frac{1}{|\Im k_{res}|}\right)$.



The Green function in the upper/lower half space takes the form

$$g^e(k;x,y) = -\frac{i}{4}\left(H_0^{(1)}(k|x-y|) + H_0^{(1)}(k|x'-y|)\right),$$

where $H_0^{(1)}$ is the first-kind Hankel function of order 0, and

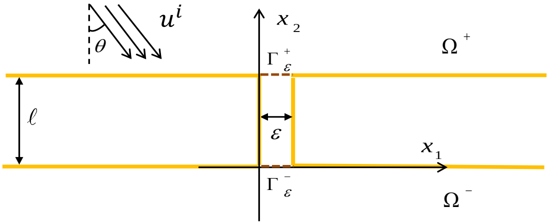
$$x' = \begin{cases} (x_1, 2-x_2) & \text{if } x,y \in \Omega^+, \\ (x_1, -x_2) & \text{if } x,y \in \Omega^-. \end{cases}$$

The Green function in the domain S_ε takes the form:

$$g_\varepsilon^i(k;x,y) = \sum_{m,n=0}^{\infty} c_{mn}\phi_{mn}(x)\phi_{mn}(y),$$

where $c_{mn} = \dfrac{1}{k^2-(m\pi/\varepsilon)^2-(n\pi)^2}$, $\phi_{mn}(x) = \sqrt{\dfrac{\alpha_{mn}}{\varepsilon}}\cos\left(\dfrac{m\pi x_1}{\varepsilon}\right)\cos(n\pi x_2)$, and

$$\alpha_{00} = 1; \quad \alpha_{0m} = \alpha_{m0} = 2 \text{ for } m \geq 1; \quad \alpha_{mn} = 4 \text{ for others.}$$



- Wave field above and below the metal slab:

$$u_\varepsilon(x) = \int_{\Gamma_\varepsilon^+} g^e(x,y)\frac{\partial u_\varepsilon}{\partial \nu} ds_y + u^i + u^r, \quad x \in \Omega^+.$$

$$u_\varepsilon(x) = \int_{\Gamma_\varepsilon^-} g^e(x,y)\frac{\partial u_\varepsilon}{\partial \nu} ds_y \quad x \in \Omega^-.$$

- Wave field in the slit S_ε: $u_\varepsilon(x) = -\int_{\Gamma_\varepsilon^+\cup\Gamma_\varepsilon^-} g_\varepsilon^i(x,y)\frac{\partial u_\varepsilon}{\partial \nu} ds_y$.
- Integral equation formulation:

$$\begin{cases} \int_{\Gamma_\varepsilon^+}\left(-\frac{i}{2}\right)H_0^{(1)}(k|x-y|)\frac{\partial u_\varepsilon}{\partial \nu}ds_y + \int_{\Gamma_\varepsilon^+\cup\Gamma_\varepsilon^-} g_\varepsilon^i(x,y)\frac{\partial u_\varepsilon}{\partial \nu}ds_y = -(u^i+u^r), & \text{on } \Gamma_\varepsilon^+, \\ \int_{\Gamma_\varepsilon^-}\left(-\frac{i}{2}\right)H_0^{(1)}(k|x-y|)\frac{\partial u_\varepsilon}{\partial \nu}ds_y + \int_{\Gamma_\varepsilon^+\cup\Gamma_\varepsilon^-} g_\varepsilon^i(x,y)\frac{\partial u_\varepsilon}{\partial \nu}ds_y = 0, & \text{on } \Gamma_\varepsilon^-. \end{cases}$$

Integral Equation Formulation III: scaling

- Scaling by ε: Let $x_1 = \varepsilon X,\ y_1 = \varepsilon Y,\ X, Y \in (0,1)$;

$$\varphi_1(X) := -\frac{\partial u_\varepsilon}{\partial x_2}(\varepsilon X, 1),\ \varphi_2(X) := \frac{\partial u_\varepsilon}{\partial x_2}(\varepsilon X, 0),\ f(X) := (u^i + u^r)(\varepsilon X, 1);$$

$$G^e_\varepsilon(X,Y) := g^e_\varepsilon(\varepsilon X, 1; \varepsilon Y, 1) = g^e_\varepsilon(\varepsilon X, 0; \varepsilon Y, 0);$$

$$G^i_\varepsilon(X,Y) := g^i_\varepsilon(\varepsilon X, 1; \varepsilon Y, 1) = g^i_\varepsilon(\varepsilon X, 0; \varepsilon Y, 0);$$

$$\tilde{G}^i_\varepsilon(X,Y) := g^i_\varepsilon(\varepsilon X, 1; \varepsilon Y, 0) = g^i_\varepsilon(\varepsilon X, 0; \varepsilon Y, 1).$$

- Equivalent integral equation formulation:

$$\begin{bmatrix} T^e + T^i & \tilde{T}^i \\ \tilde{T}^i & T^e + T^i \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} = \begin{bmatrix} f/\varepsilon \\ 0 \end{bmatrix}.$$

where

$$(T^e \varphi)(X) = \int_0^1 G^e_\varepsilon(X,Y)\varphi(Y)dY \quad X \in (0,1);$$

$$(T^i \varphi)(X) = \int_0^1 G^i_\varepsilon(X,Y)\varphi(Y)dY \quad X \in (0,1);$$

$$(\tilde{T}^i \varphi)(X) = \int_0^1 \tilde{G}^i_\varepsilon(X,Y)\varphi(Y)dY \quad X \in (0,1).$$

Asymptotic Expansions for the Integral Operators

- Asymptotic expansions of the kernels:

$$
\begin{aligned}
G^e_\varepsilon(X,Y) &= \frac{1}{\pi}\left[\ln\varepsilon+\ln k+\gamma_0\right]+\frac{1}{\pi}\ln|X-Y|+O((\varepsilon|X-Y|)^2\ln(\varepsilon|X-Y|);\\
G^i_\varepsilon(X,Y) &= \frac{\cot k}{k\varepsilon}+\frac{2\ln 2}{\pi}+\frac{1}{\pi}\left[\ln\left(\left|\sin\left(\frac{\pi(X+Y)}{2}\right)\right|\right)+\ln\left(\left|\sin\left(\frac{\pi(X-Y)}{2}\right)\right|\right)\right]\\
&\quad +O(k^2\varepsilon^2);\\
\tilde{G}^i_\varepsilon(X,Y) &= \frac{1}{(k\sin k)\varepsilon}+O\left(e^{-1/\varepsilon}\right).\\
\kappa(X,Y) &= \frac{1}{\pi}\left[\ln\left(\left|\sin\left(\frac{\pi(X-Y)}{2}\right)\right|\right)+\ln\left(\left|\sin\left(\frac{\pi(X+Y)}{2}\right)\right|\right)+\ln|X-Y|\right].
\end{aligned}
$$

- Asymptotic expansions of the integral operators:

$$
\begin{bmatrix} T^e+T^i & \tilde{T}^i \\ \tilde{T}^i & T^e+T^i \end{bmatrix} = \begin{bmatrix} \beta & \tilde{\beta} \\ \tilde{\beta} & \beta \end{bmatrix} P + K\mathbb{I} + \begin{bmatrix} K_\infty & \tilde{K}_\infty \\ \tilde{K}_\infty & K_\infty \end{bmatrix} =: \mathbb{P}+\mathbb{L}.
$$

where K is the integral operator corresponding to the Schwarz kernel $\kappa(X,Y)$ and

$$
\begin{aligned}
\beta(k,\varepsilon) &= \frac{\cot k}{k\varepsilon}+\frac{1}{\pi}(2\ln 2+\ln k+\gamma_0)+\frac{1}{\pi}\ln\varepsilon, \qquad \tilde{\beta}(k,\varepsilon)=\frac{1}{(k\sin k)\varepsilon}\\
P\varphi(X) &= (\varphi,\chi_{(0,1)})\chi_{(0,1)}.
\end{aligned}
$$

Let I be a bounded open interval in $\mathbf{R}$ and define

$$H^s(I) := \{u = U|_I \mid U \in H^s(\mathbf{R})\}.$$

Then $H^s(I)$ is a Hilbert space with the norm

$$\|u\|_{H^s(I)} = \inf\{\|U\|_{H^s(\mathbf{R})} \mid U \in H^s(\mathbf{R}) \text{ and } U|_I = u\}.$$

We also define

$$\tilde{H}^s(I) := \{u = U|_I \mid U \in H^s(\mathbf{R}) \text{ and } supp\, U \subset \bar{I}\}.$$

The space $\tilde{H}^s(I)$ is the dual of $H^{-s}(I)$ and the norm for $\tilde{H}^s(I)$ can be defined via the duality. For simplicity, we denote $V_1 = \tilde{H}^{-\frac{1}{2}}(0,1)$ and $V_2 = H^{\frac{1}{2}}(0,1)$.

Lemma

The operator K is bounded from V_1 to V_2 with a bounded inverse. Moreover,

$$\alpha := \langle K^{-1}1, 1\rangle \neq 0.$$

- Look for k such that $(\mathbb{P}+\mathbb{L})\varphi = 0$ attains non-trivial solutions (characteristic value of the operator-valued function $\mathbb{P}+\mathbb{L}$).
- The operator equation reduces to

$$(\mathbb{M}+\mathbb{I}) \begin{bmatrix} \langle \varphi, \mathbf{e}_1 \rangle \\ \langle \varphi, \mathbf{e}_2 \rangle \end{bmatrix} = 0,$$

where $\mathbf{e}_1 = [1,0]^T$ and $\mathbf{e}_2 = [0,1]^T$, and the matrix

$$\mathbb{M} = \left(\beta \mathbb{I} + \tilde{\beta} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \cdot \begin{bmatrix} \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_1 \rangle & \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_2 \rangle \\ \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_2 \rangle & \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_1 \rangle \end{bmatrix}$$

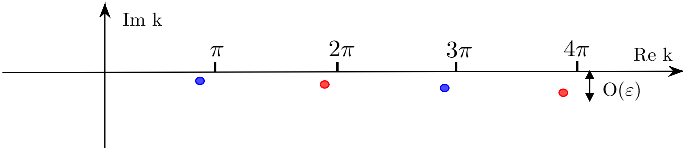
- The eigenvalues of $\mathbb{M}+\mathbb{I}$ are given by

$$\lambda_1(k,\varepsilon) = 1 + (\beta(k,\varepsilon) + \tilde{\beta}(k,\varepsilon)) \left(\langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_1 \rangle + \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_2 \rangle \right),$$
$$\lambda_2(k,\varepsilon) = 1 + (\beta(k,\varepsilon) - \tilde{\beta}(k,\varepsilon)) \left(\langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_1 \rangle - \langle \mathbb{L}^{-1}\mathbf{e}_1, \mathbf{e}_2 \rangle \right).$$

Resonance condition

The resonances are the roots of $\lambda_1(k,\varepsilon) = 0$ or $\lambda_2(k,\varepsilon) = 0$.

Asymptotic Expansions for Resonances



Theorem

The following asymptotic expansions hold for the resonances of the scattering problem:

$$k_{m,1}=(2m-1)\pi+2(2m-1)\pi\left[\frac{1}{\pi}\varepsilon\ln\varepsilon+\left(\frac{1}{\alpha}+\frac{1}{\pi}(2\ln 2+\ln((2m-1)\pi)+\gamma_0)\right)\varepsilon\right]$$
$$+O(\varepsilon^2\ln^2\varepsilon),$$
$$k_{m,2}=2m\pi+4m\pi\left[\frac{1}{\pi}\varepsilon\ln\varepsilon+\left(\frac{1}{\alpha}+\frac{1}{\pi}(2\ln 2+\ln(2m\pi)+\gamma_0)\right)\varepsilon\right]+O(\varepsilon^2\ln^2\varepsilon),$$

for $m=1,2,3,\cdots$, and $m\varepsilon\ll 1$. Here $\alpha=\langle K^{-1}1,1\rangle$, $\gamma_0=c_0-\ln 2-i\pi/2$, and c_0 is the Euler constant.

Remark The imaginary part of each resonance has an order of $O(\varepsilon)$.

Solution of the Integral Equation at Resonant Frequencies

- Solving the operator equation $(\mathbb{P}+\mathbb{L})\varphi = \mathbf{f}$ yields

$$\varphi \quad = \quad K^{-1}1 \cdot \left[d_1 \cdot O(k) \cdot \mathbf{e}_1 + \frac{\alpha}{\varepsilon \cdot \lambda_1}(\mathbf{e}_1 + \mathbf{e}_2) + \frac{\alpha}{\varepsilon \cdot \lambda_2}(\mathbf{e}_1 - \mathbf{e}_2) \right] + \text{H.O.T},$$

  where $\alpha = \langle K^{-1}1, 1 \rangle$.

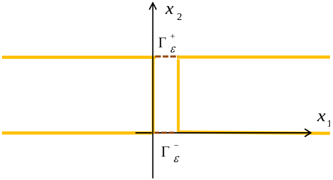
- Away from the resonant frequencies, $\lambda_1 \sim O\left(1/\varepsilon\right)$, $\lambda_2 \sim O\left(1/\varepsilon\right)$, and consequently $\varphi \sim O(1)$.

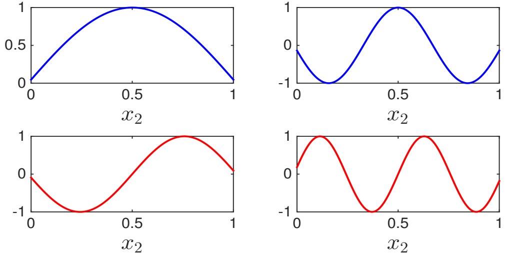
Solution at resonant frequencies

At the odd and even resonant frequencies $k = \Re k_{m,1}$ and $k = \Re k_{m,2}$,

$$\lambda_1 = -\frac{i\alpha}{2} + O(\varepsilon \ln^2 \varepsilon), \quad \lambda_2 = -\frac{i\alpha}{2} + O(\varepsilon \ln^2 \varepsilon).$$

Field Enhancement at Resonant Frequencies: In the Slit





The wave field inside the slit adopts the following expansion at the odd and even resonances respectively:

$$u_\varepsilon(x) = \frac{1}{\varepsilon} \cdot \frac{2i}{k\sin(k/2)} \cdot \cos(k(x_2 - 1/2)) + O(\ln^2 \varepsilon)$$

and

$$u_\varepsilon(x) = -\frac{1}{\varepsilon} \cdot \frac{2i}{k\cos(k/2)} \cdot \sin(k(x_2 - 1/2)) + O(\ln^2 \varepsilon).$$

Field Enhancement at Resonant Frequencies: Over Slit Apertures

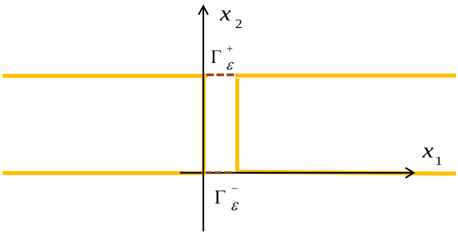
On the aperture Γ_ε^+, the wave field adopts the following expansion at resonant frequencies:

$$u_\varepsilon(x_1, 1) = -\frac{2i}{\pi}\ln\varepsilon + O(1)$$

On the aperture Γ_ε^-,

$$u_\varepsilon(x_1, 0) = -\frac{2i}{\pi}\ln\varepsilon + O(1) \quad \text{and} \quad u_\varepsilon(x_1, 0) = \frac{2i}{\pi}\ln\varepsilon + O(1).$$

at odd and even resonant frequencies, respectively.

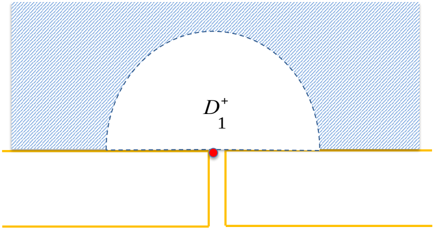


Field Enhancement at Resonant Frequencies: Far Field

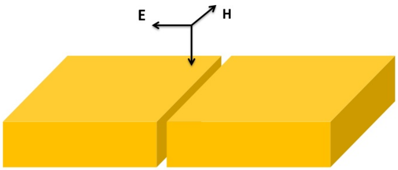
In the region $\Omega^+ \backslash D_1^+$, the scattered field adopts the following expansion at resonant frequencies:

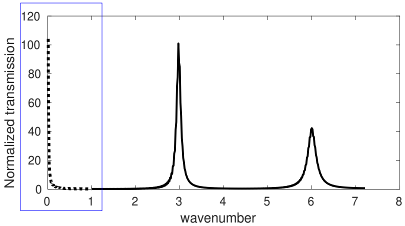
$$u_\varepsilon^s(x) = -2i \cdot g^e(x,(0,1)) + O(\varepsilon \ln^2 \varepsilon).$$

Remark The amplitude of the wave at resonant frequencies: $O(\frac{1}{\sqrt{|x|}})$.



Non-resonant Enhancement at Low Frequencies I





- Estimation (L-Reitich, 2015): $\frac{\underline{C}_E}{k} \le \frac{||E_\varepsilon||_{L^2(S_\varepsilon)}}{||E^i||_{L^2(S_\varepsilon)}} \le \frac{\overline{C}_E}{k}$, $\underline{C}_H \le \frac{||H_\varepsilon||_{L^2(S_\varepsilon)}}{||H^i||_{L^2(S_\varepsilon)}} \le \overline{C}_H$
- Expand the wave field in the slit as the sum of wave-guide modes:

$$u_\varepsilon(x) = a_0 \cos kx_2 + b_0 \cos k(1-x_2) + \sum_{m\ge1} \left[a_m \exp\left(-k_2^{(m)} x_2\right) + b_m \exp\left(-k_2^{(m)}(1-x_2)\right)\right] \cos\frac{m\pi x_1}{\varepsilon},$$

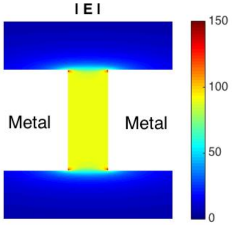
where $k_2^{(m)} = \sqrt{(m\pi/\varepsilon)^2 - k^2}$.

Lemma

$$a_0 = \frac{1}{k\sin k}\Big[\alpha + O(k\varepsilon)\Big]\cdot\left(\frac{1}{\varepsilon\cdot\lambda_1} + \frac{1}{\varepsilon\cdot\lambda_2}\right), \quad b_0 = \frac{1}{k\sin k}\Big[\alpha + O(k\varepsilon)\Big]\cdot\left(\frac{1}{\varepsilon\cdot\lambda_1} - \frac{1}{\varepsilon\cdot\lambda_2}\right),$$

$$\sqrt{m}\,|a_m| \le C, \quad \sqrt{m}\,|b_m| \le C, \quad \text{for } m \ge 1,$$

Non-resonant Enhancement at Low Frequencies II: In the Slit



- If $k \ll 1$ and $\varepsilon \ll 1$,

$$u_\varepsilon = 2x_2 + O(k^2) + O(\varepsilon \ln \varepsilon).$$

- The electric field

$$E_{\varepsilon,1} = \frac{2}{k\sqrt{\tau_0/\mu_0}} + O(k^2) + O(\varepsilon \ln \varepsilon);$$

$E_{\varepsilon,2} \sim O(\varepsilon)$ and $E_{\varepsilon,2} \sim o(\varepsilon)$ near and away from apertures.

Theorem

No significant magnetic field enhancement is gained. However, the electric field $|E_\varepsilon| \sim O(1/k)$ or $|E_\varepsilon| \sim O(1/(k\ell))$ if $\ell \neq 1$.

$|E_\varepsilon|/|E^{inc}|$ for $k = 0.1$. Left: $\ell = 0.1$, $\varepsilon = 0.01$; Right: $\ell = 0.01$, and $\varepsilon = 0.001$.